

# Eric C. Cyr

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CONTACT INFORMATION      University of Illinois at Urbana-Champaign      <http://www.cse.uiuc.edu/~ericcyr>  
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EDUCATION      **University of Illinois at Urbana-Champaign**, Urbana, Illinois  
Ph.D. in Computer Science (in progress),  
August 2003-Present (Expected graduation: Summer 2008)  
Thesis Advisor: Stephen Bond

**Clemson University**, Clemson, South Carolina  
B.S. in Computer Science,  
Graduation: December 2002, *Summa Cum Laude*

RESEARCH INTERESTS      Numerical Analysis, Scientific Computing, Computational Chemistry, Computational Biology, Poisson-Boltzmann Equation, Potential of Mean Force Calculations, Software Design and Development.

EXPERIENCE      **University of Illinois at Urbana-Champaign**, Urbana, Illinois      Aug. 2003-Present  
*Research Assistant:* Department of Computer Science  
Research area: Potential of Mean Force Calculations, Poisson-Boltzmann Equation

**Clemson University**, Clemson, South Carolina      Jan. 2003-July 2003  
*Research Programmer:* Center for Advanced Engineering Fibers and Films  
Research area: High Performance C++ Software for Non-Newtonian Fluids

**Sandia National Laboratories**, Albuquerque, New Mexico      Summer 2002  
*Summer Intern:* Computer Science Research Institute  
Research area: Initial development of "Surfpack" software for surrogate modeling

**Schlumberger Industries**, West Union, South Carolina      May 1999-Dec. 2000  
*Test Engineering Co-op*

PROJECTS      **Potential of Mean Force**  
The Potential of Mean Force is the free energy profile computed from a coarse grained description of a (bio)molecular system. This research focuses on numerical methods for computing the profile. Approaches include methods based on solving boundary value problems [1] and approximation of probability density functions using maximum entropy methods.

**Poisson-Boltzmann Equation**  
Simulating a molecule requires accurate representation of the solvent. The electrostatic forces of the solvent on the molecule can be modeled implicitly by a nonlinear PDE known

as the Poisson-Boltzmann equation. Algorithms for solving the Poisson-Boltzmann equation were studied, including goal oriented adaptive mesh refinement and multigrid methods.

### **Fast Electrostatics with a Smoothly Varying Dielectric**

Performed initial study of solving the Poisson equation for the electrostatic potential surrounding a molecular system with a dielectric that varies smoothly around the molecule. This relies on computing the effective charge distribution induced by the dielectric using fast linear time methods.

### **Generic Programming for Non-Newtonian Viscoelastic Flows**

Implemented a finite element code for viscoelastic flows exploiting the generic programming abilities of C++. Investigated fast and modular techniques for implementation of finite elements. The resulting code's run time is competitive with a similar package written in FORTRAN [3].

### **Surface Fitting Software Package**

Under the supervision of Anthony Giunta at (Sandia National Laboratories) I designed a software package for surface fitting methods. This package was required to be accessible to both C++ software and to FORTRAN software [2].

## PUBLICATIONS

- [1] E.C. Cyr and S.D. Bond, Using the Method of Weighted Residuals to Compute Potentials of Mean Force, *Journal of Computational Physics*, 225:714-729, 2007.
- [2] A.A. Giunta, L.P. Swiler, S.L. Brown, M.S. Eldred, M.D. Richards, and E.C. Cyr, "The Surfpack Software Library for Surrogate Modeling of Sparse Irregularly Spaced Multidimensional Data," in *Proceedings of the 11th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*, AIAA Paper 2006-7049, Portsmouth, VA, 2006.
- [3] C.L. Cox, E.C. Cyr, E.B. Duffy, J.B. von Oehsen, and B.A. Malloy, An Efficient C++ Finite Element Viscoelastic Flow Code Exploiting Generative Programming Techniques, *Luxferm 2003 International Conference on Finite element for process*, Luxembourg, Nov. 13-14, 2003.
- [4] J.B. von Oehsen, C.L. Cox, E.C. Cyr, and B.A. Malloy, Using Design Patterns and XML to Construct an Extensible Finite Element System, *Proceedings of the International Conference on Computational Science*, Part III, April 21-24, 2002, Lecture Notes in Computer Science, 2331, Springer-Verlag 2002, pp. 735-744.
- [5] J.B. von Oehsen, E.C. Cyr, C.L. Cox, and B.A. Malloy, An Internet-Accessible Software Package for Modeling Viscoelastic Flow, *Internet Accessible Mathematical Computation 2002 Workshop*, Lille France, July 7, 2002.

## PRESENTATIONS

E. C. Cyr and S. D. Bond, A Comparison of Maximum Likelihood and Weighted Residual Approximations to the Potential of Mean Force, Minneapolis, MN, *IMA Summer Program: Classical and Quantum Approaches in Molecular Modeling Engineering*, July 24, 2007 (Poster).

E. C. Cyr, A Numerical Study of the Regularized Poisson-Boltzmann Equation on Structured Grids, Urbana, IL, *University of Illinois at Urbana-Champaign CSE Symposium*, April

10, 2007 (Presentation).

E. C. Cyr and S. D. Bond, A Comparison of Maximum Likelihood and Weighted Residual Approximations to the Potential of Mean Force, Costa Mesa, CA, *SIAM Conference on Computational Science and Engineering*, February 2007 (Presentation).

#### SKILLS

- ◇ Proficiency in C/C++, Java, MATLAB, and Python
- ◇ Experience with Windows, Linux, Mac OS, Irix, and Solaris
- ◇ Experience with NAMD and VMD molecular simulation and visualization software

#### AWARDS

**CSE Fellow**, 2006-2007 and 2007-2008, University of Illinois at Urbana-Champaign  
An annual competitive fellowship based on a campus-wide call for interdisciplinary and computationally oriented proposals.

- 2007-2008 Title: *Fast Solutions to the Poisson-Boltzmann Equation Using Hierarchical Basis Functions* (8 selected out of 33)
- 2006-2007 Title: *Multilevel Iterative Methods for Solving the Poisson-Boltzmann Equation*

**Outstanding Junior in Computer Science**, 2002, Clemson University

#### REFERENCES

**Stephen Bond**, *Thesis Advisor*

University of Illinois at Urbana-Champaign, Department of Computer Science

Details and additional references available upon request.